

An Algorithmic and Software Framework for Applied Partial Differential Equations

Principal Investigators:

J. Bell, LBNL

D. Brown, LLNL

M. Berger, New York Univ.

P. Colella, LBNL

R. Leveque, Univ. of Washington

M. Minion, Univ. of North Carolina

G. Puckett, Univ. of California, Davis

C. Rutland, Univ. of Wisconsin

<http://davis.lbl.gov/APDEC>

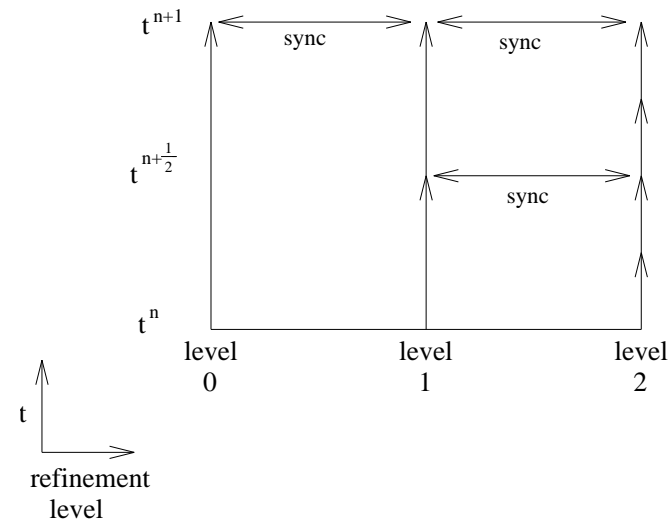
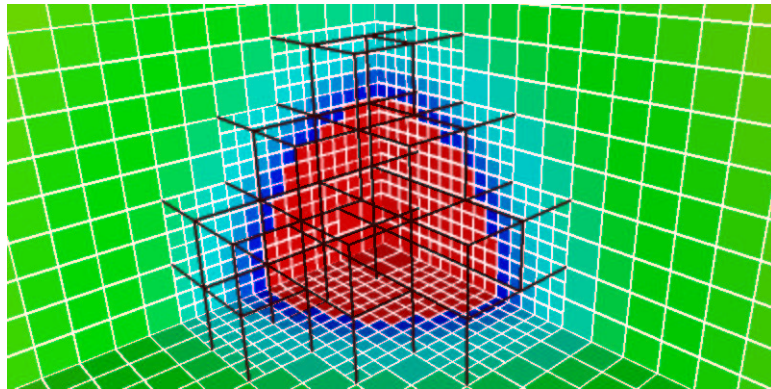
An Algorithmic and Software Framework for Applied Partial Differential Equations (APDEC)

Goals

- Development of algorithms and software for PDEs based on locally structured grids. Technologies include adaptive mesh refinement (AMR), embedded boundary representation of complex geometries, and particle methods.
- Applications development: end-to-end development of new simulation capabilities for combustion, magnetic fusion, and accelerator design.
- Software development: factorized version of LBNL AMR tools to to maximize reuse across applications (Chombo). Leverage activities in other ISICs.

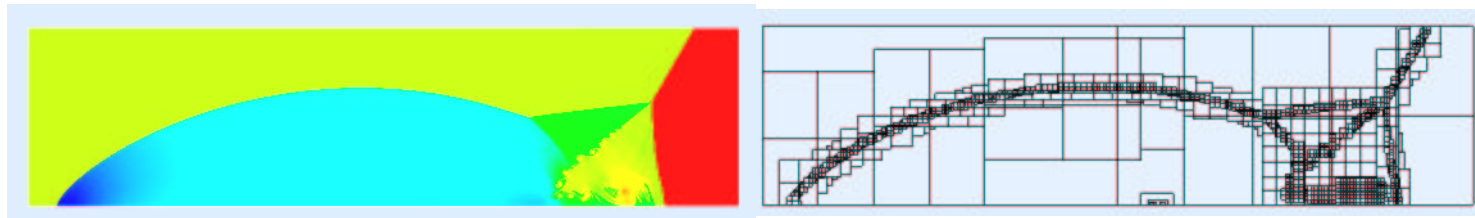
Block-Structured Local Refinement (Berger and Oliger, 1984)

Goal: adjust the computational effort locally to maintain a uniform level of accuracy throughout the problem domain.



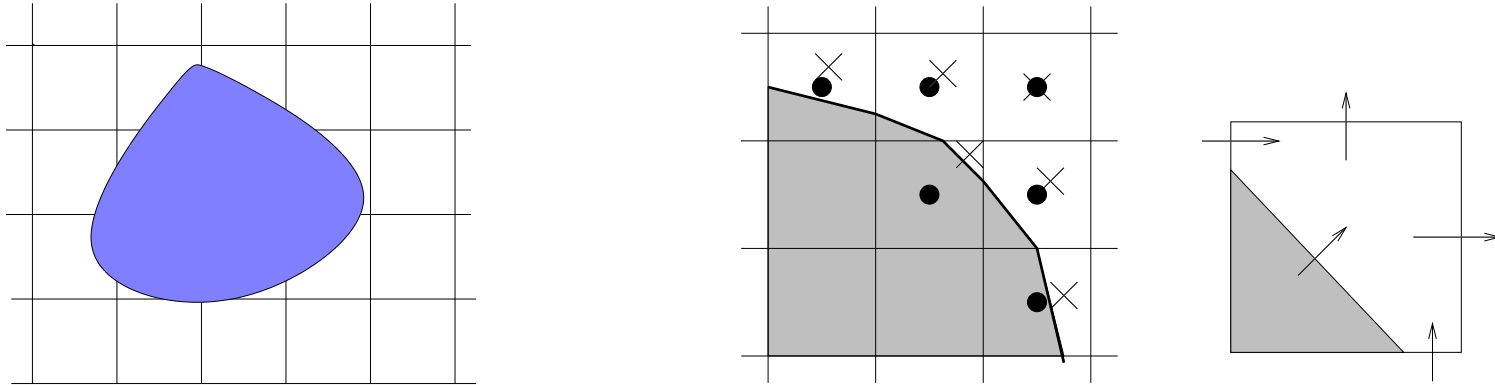
Refined regions are organized into rectangular patches.

Refinement performed in time as well as in space.



Cartesian Grid Representation of Irregular Boundaries

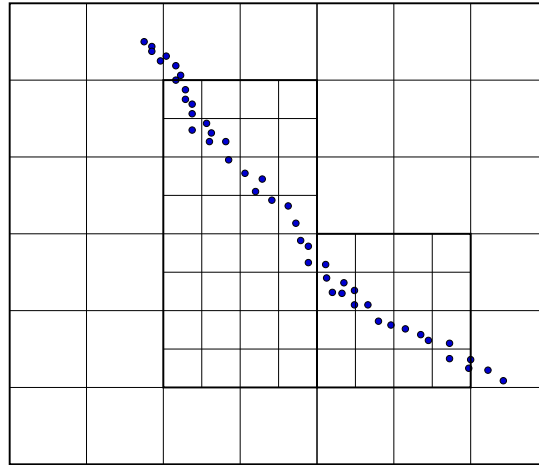
Based on nodal-point representation or finite-volume representation.



Advantages of underlying rectangular grid:

- Grid generation is tractable.
- Good discretization technology, e.g. well-understood consistency theory for finite differences. Geometric multigrid for solvers.
- Straightforward coupling to structured AMR.

Particles and AMR



Algorithmic Issues:

- Transfers of particles across coarse/fine interface boundaries
- Particle \rightarrow grid and grid \rightarrow particle transfers in the presence of refinement boundaries (modified stencils)
- preventing self-induced effects.

Software Approach

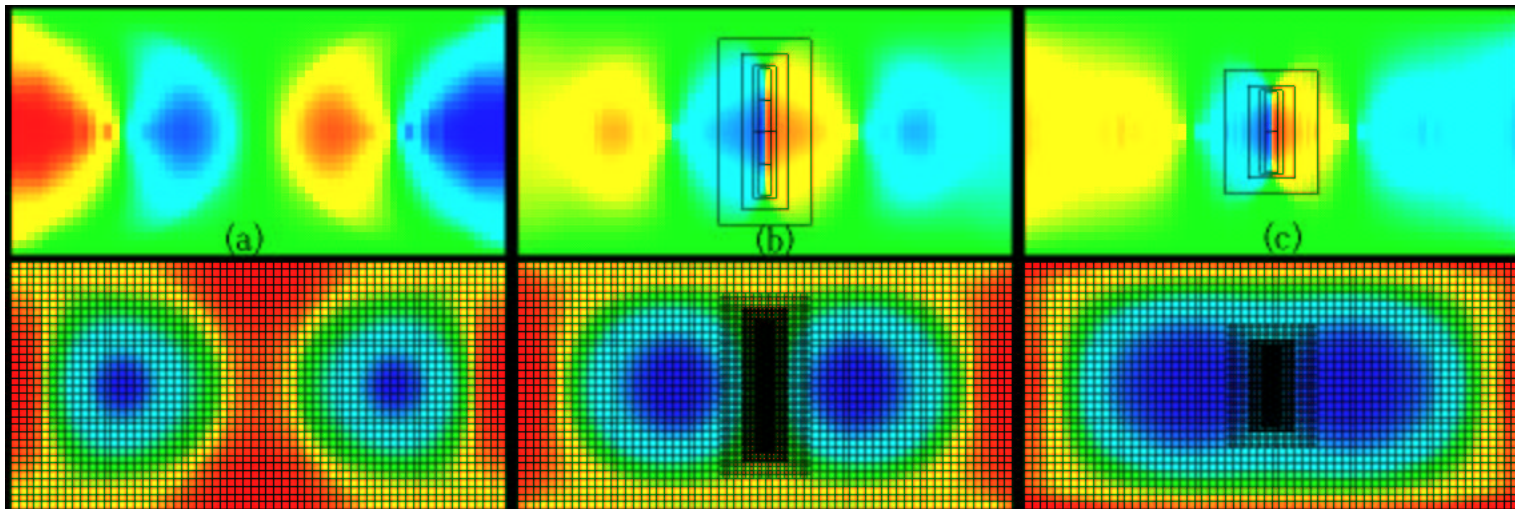
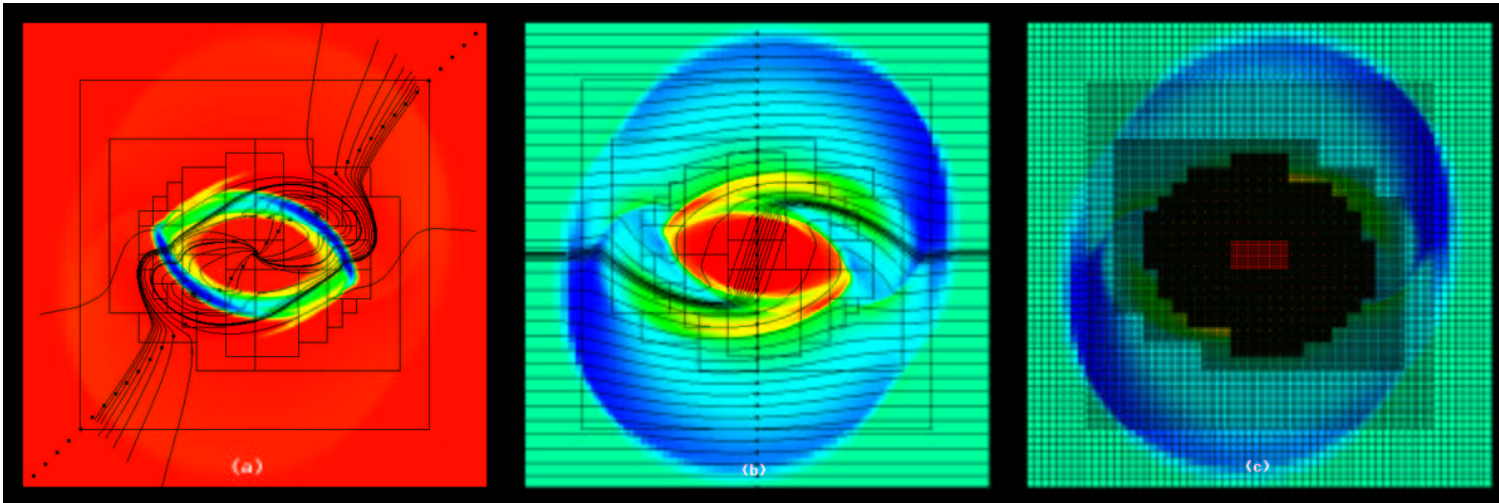
Requirement: to support a wide variety of applications that use block-structured AMR using a common software framework.

- Mixed-language model: C++ for higher-level data structures, Fortran for regular single-grid calculations.
- Reuseable components. Component design based on mapping of mathematical abstractions to classes.
- Build on public-domain standards: MPI, HDF5, VTK.
- Interoperability with other SciDAC ISIC tools: grid generation (TSTT), solvers (TOPS), performance analysis tools (PERC).

Applications Progress

- Combustion. Developed AMR codes in 2D and 3D for low Mach number combustion with complex chemistry, realistic diffusive transport. Obtained quantitative agreement of 2D laminar diffusion flame calculations with experimental NO_x measurements. Performed 3D time-dependent simulation capability of laboratory-scale turbulent methane flames (AMR + low Mach number leads to 10^4 reduction in compute time over standard compressible DNS).
- Magnetic Fusion. Developed explicit and semi-implicit AMR algorithms for resistive MHD in two and three dimensions. Performed high-resolution simulations of magnetic reconnection problem.
- Accelerator Modeling. Developed 3D AMR code for Poisson's equation with Shortley-Weller representations of irregular conducting boundaries. Developed preliminary implementation of AMR PIC code, and coupled to MaryLie / IMPACT beam dynamics code.

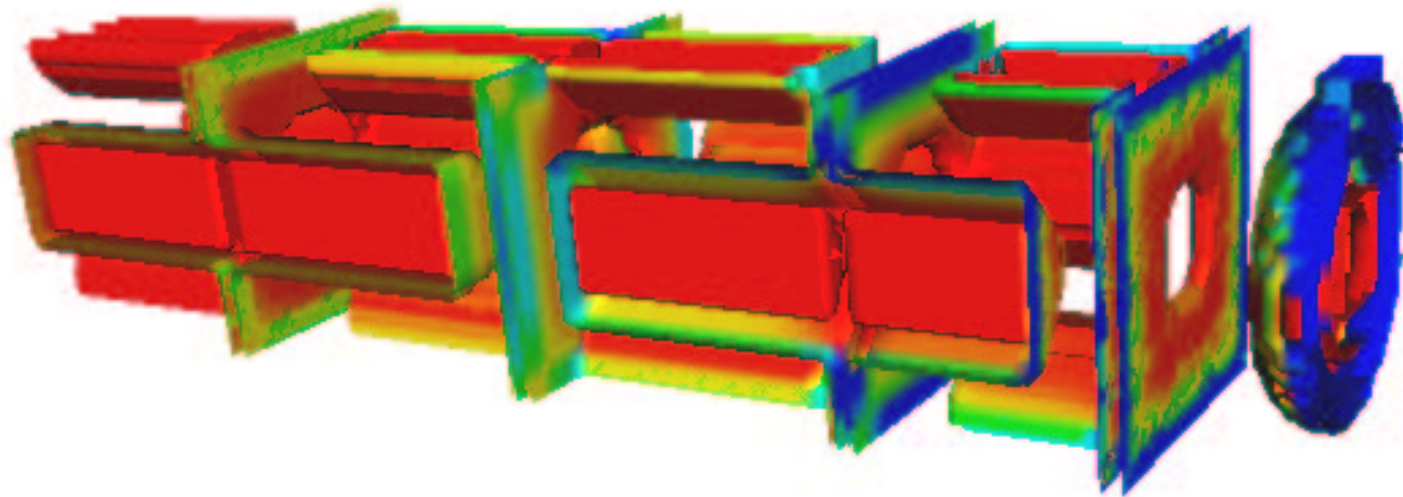
AMR for Magnetohydrodynamics (R. Samtaney, PPPL)



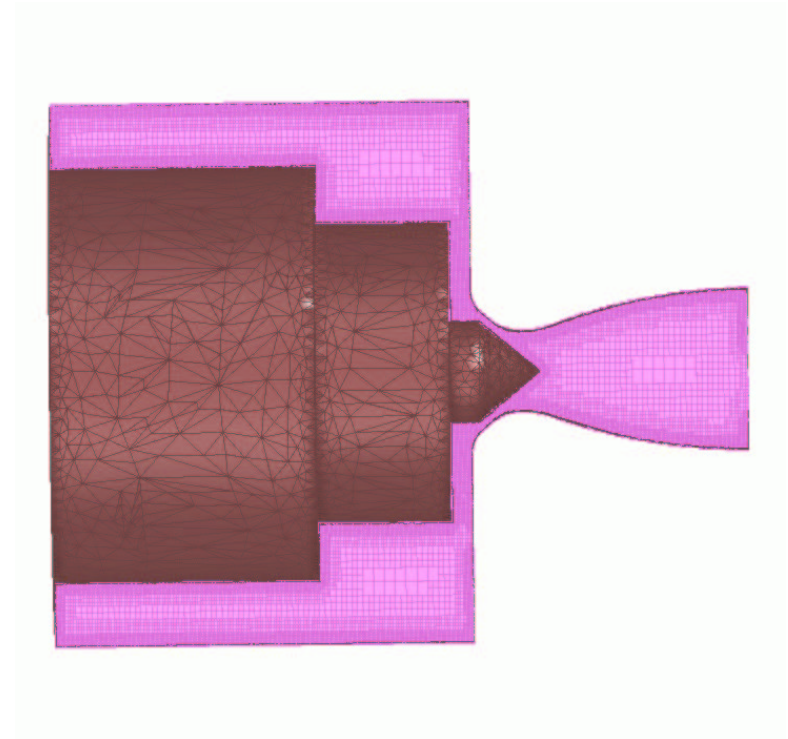
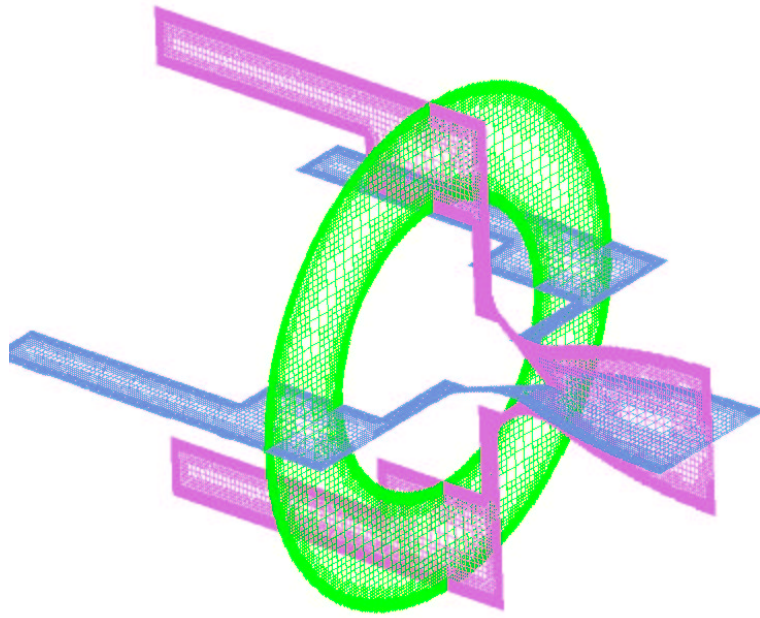
Algorithmic and Software Progress

- Improvements to Chombo package for AMR applications, including variable coefficient elliptic solvers, support for periodic boundary conditions, and new general-purpose hyperbolic drivers. Support for AMR particle methods.
- New stable and robust embedded boundary algorithms and solvers for PDEs in complex geometries.
- New tools for grid generation for embedded boundary calculations (joint with TSTT).
- Interoperability tools: framework-neutral AMR data alias; interface to HDF5 I/O, ChomboVis AMR visualization tools. Chombo interface to *hypre* structured-grid linear solver package from TOPS. Chombo interface to PAPI performance measurement tools from PERC.
- New semi-implicit spectral deferred corrections algorithms for complex time-dependent problems.

AMR Shortley-Weller Solver for Poisson's Equation.



**Grid Generation for AAC Gas Jet Simulation Using Cart3D (M. Berger (NYU),
A. Petersson (LLNL), C. Geddes (LBNL))**



Future Plans - Near Term

- Combustion: comparison of 3D turbulent flame calculations to laboratory-scale flame experiments of Cheng, et. al.; coupling of spray models to AMR.
- Magnetic fusion: develop AMR code capability for pellet injection problem. Coupling of semi-implicit methods to models for reconnection.
- Accelerator modeling: development of AMR-PIC codes for beam dynamics based on alternative formulations. Fast evaluation version of James' method for infinite domain boundary conditions. Complete development of gas-jet simulation capability for laser-driven plasma-wakefield accelerators.
- Software: Complete development of embedded boundary AMR capability. Performance tuning of Chombo, e.g. introduction of level-based stencil operations, alternative grid generation, load-balancing strategies. Run-time grid generation for embedded boundaries. Demonstration project of componentization of Chombo elliptic solvers (joint with CCTTSS).

Long-Term Plans / Opportunities

- Development of AMR allspeed algorithms for low-Mach number / locally anelastic problems (combustion, supernova combustion, magnetic fusion).
- Combustion: extension to more complete nitrogen chemistry. Combustion in complex geometries.
- Extension of Cartesian grid methods to free boundaries, non-unit aspect ratios, other orthogonal coordinate systems (tracked flame fronts, plasma boundary in tokamak / stellarator geometries, gas jet boundary).
- Development of new algorithms / solvers for AMR grids: analysis-based scalable solvers for constant-coefficient problems, Newton-Krylov-Schwartz methods, conservative higher-order solvers (accelerator modeling, magnetic fusion).
- AMR for 5D / 6D phase space, hybrid fluid-kinetic modeling, Maxwell-Vlasov (accelerator modeling, magnetic fusion).